

Theoretical Ambiguities of QCD Predictions at the Z^0 Peak*

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Abstract

We discuss uncertainties of QCD predictions for the hadronic width of the Z^0 boson. Emphasis is put on quantitative estimates, taking into account the current precision of experimental data.

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1 Introduction

The hadronic width of the Z^0 boson, $\Gamma_h \equiv \Gamma(Z^0 \rightarrow \text{hadrons})$, or the ratio

$$R_Z \equiv \frac{\Gamma_h}{\Gamma_0}, \quad \Gamma_0 \equiv \frac{G_F M_Z^3}{2\pi\sqrt{2}}, \quad (1)$$

which is closely related to the familiar ratio R in e^+e^- annihilations into hadrons, provide theoretically very clear conditions for the verification of perturbative QCD. This is due to several favourable circumstances:

- nonperturbative power corrections are expected to be negligible at the scale M_Z
- perturbative corrections are calculated up to next-to-next-to-leading order (NNLO)
- the dependence of perturbative expansion for (1) on the choice of the renormalization scheme (RS) is weak
- in calculating QCD corrections to (1) the running α_s can be taken as that corresponding to five effectively massless quarks, $\alpha_s^{(5)}$
- the effects of the finite bottom quark mass on the expansion coefficients of Γ_h in this couplant $\alpha_s^{(5)}$ have been calculated up to the NLO
- the explicit dependence of Γ_h on the top quark mass m_t has been calculated in the large m_t expansion up to the NNLO
- the statistics of the data is large, and thus the experimental accuracy rather high, in particular compared with the closely related process of e^+e^- annihilations into hadrons.

On the other hand, at the scale M_Z the magnitude of QCD corrections to the basic electroweak decay mechanism is smaller than for quantities at lower energy scales, such as the τ -lepton semileptonic decay width and therefore more difficult to pin down. In this part of the paper we give quantitative estimates of some of the above-mentioned uncertainties and address the related question: assuming the validity of QCD and taking into account these uncertainties, how accurately can the basic QCD parameter α_s be determined?

As any meaningful discussion of the quantitative importance of higher order QCD corrections depends on the ability of experiments to ‘see’ them, we start by recalling the relevant experimental data [1]:

$$M_Z = 91.187 \pm 0.007 \text{ GeV} \quad (2)$$

$$\Gamma_0 = 0.99528 \pm 0.00023 \text{ GeV} \quad (3)$$

$$\Gamma_h = 1.7407 \pm 0.0059 \text{ GeV}, \quad (4)$$

which imply the following relative errors, relevant for further discussion

$$\frac{\Delta\Gamma_0}{\Gamma_0} = 2.3 \cdot 10^{-4}, \quad \frac{\Delta\Gamma_h}{\Gamma_h} \doteq \frac{\Delta R_Z}{R_Z} = 3.5 \cdot 10^{-3}. \quad (5)$$

Note that the precision $\Delta\Gamma_0$ of the determination of Γ_0 is more than an order of magnitude better than that of Γ_h and can thus be neglected with respect to $\Delta\Gamma_h$.

Because the dominant part of perturbative QCD predictions for Γ_h has the same generic form as does R_Z , i.e.,

$$A \left[1 + \frac{\alpha_s}{\pi} \left(1 + r_1 \frac{\alpha_s}{\pi} + \dots \right) \right], \quad (6)$$

and $\alpha_s(M_Z)/\pi \doteq 0.037$, these errors allow $\alpha_s(M_Z)$ to be determined to within about 8.5% accuracy. Translated into the sensitivity to Λ , this amounts to a factor of 1.9 uncertainty. Improving further the accuracy of the data by a factor of two would allow it to be extracted with an error of only 36%.

2 The RS dependence: general considerations

Over the last 15 years the problem of the renormalization scheme dependence of finite order approximants to perturbation expansions in QCD (and other theories) has been the subject of lively and sometimes even heated debate. From time to time a ‘resolution’ of this problem is announced, but invariably it turns out that these ‘solutions’ contain the original ambiguity in some guise or another. We intend to provide a concise and balanced review of all the various approaches to this problem, but emphasize at the very beginning that, in our view, there is no clear winner. Nevertheless, as the dependence of finite order perturbation expansions on the choice of RS is a very real phenomenological problem, which cannot be ignored, we think the right question in this context is: How sensitive are these approximations to the choice of RS? But even in this question there hides a catch, as to give it a concrete meaning we first have to define the set of ‘allowed’ RS. The point is that without some restriction on the considered RS we could get essentially any result we want. But again, as the selection of the ‘allowed’ RS is inevitably a subjective matter and may, moreover, depend on the quantity in question, the best we can do is choose a couple of approaches which are sufficiently general, have some rationale behind them and define the theoretical ‘error’ with respect to this set of RS.

Whether the theoretical error of some quantity should be considered large or small is, of course, not given a priori, but depends on the accuracy of experimental data to which it is compared. These experimental errors for the quantities related to the Z^0 decay were estimated in the preceding section.

In this section only the RS dependence of physical quantities will be discussed. For unphysical quantities, such as the Green functions with anomalous dimensions, the situation is more complicated and some of the approaches are not directly applicable. This, however, is not a serious limitation, as what we are actually interested in are clearly only the physical quantities.

Furthermore, we shall consider only the case of QCD with n_f massless quark flavours. The reasons for this restriction are twofold. First, the relations resulting from the renormalization group (RG) considerations and expressing the internal consistency of the renormalized perturbation theory, have yet to be worked out for the general massive case. The lack of such relations precludes the general quantitative discussion of the RS dependence

problem, possible in the massless case. In the Z^0 mass range, however, we can with great accuracy consider QCD with five effectively massless quark flavours. This statement is quantified in Section 3.

In the following subsections we first discuss the quantitative description of the freedom connected with the choice of the RS ('kinematics' of the RS dependence problem) and then briefly review several of the approaches to choosing one of these RS ('dynamics' of the RS problem). We emphasize this distinction, as the two aspects are frequently mixed up. Only the latter aspect is really of substance, the former being merely a matter of convention and bookkeeping.

2.1 The description of the RS dependence

Consider the generic perturbation expansion for the physical quantity of the form

$$r(Q) = a(\text{RS}) \left[r_0 + r_1(Q, \text{RS})a(\text{RS}) + r_2(Q, \text{RS})a^2(\text{RS}) + \dots \right]; \quad r_0 = 1, \quad (7)$$

which appears in the expression for Γ_h and (1). Q in (7) denotes generically some external momentum on which r depends¹ and $a(\text{RS})$ is the *renormalized couplant* $a \equiv \alpha_s/\pi$ (the adjective renormalized will be dropped in the following). There are many different ways to quantify the dependence of such physical quantities on the RS. As a matter of convention, we shall adopt the one suggested in Ref. [2]. First, we should define the meaning of the renormalization scheme itself. In massless QCD there must be some parameter with the dimension of the mass, for the moment loosely denoted as Λ , that sets the basic scale of the theory. Once this parameter is given, any quantity can in principle be calculated as a concrete number. For a given Λ , fixing the RS means specifying the values of all perturbative coefficients $r_k(\text{RS})$, as well as the value of the expansion parameter $a(\text{RS})$ itself.

The labelling of the RS suggested in Ref. [2] starts with the familiar equation

$$\frac{da(\mu, \text{RS})}{d \ln \mu} \equiv \beta(a) = -ba^2(\mu, \text{RS}) \left(1 + ca(\mu, \text{RS}) + c_2a^2(\mu, \text{RS}) + \dots \right), \quad (8)$$

expressing the dependence of a on the scale μ , which inevitably appears in the theory during the process of renormalization. The first two coefficients on the r.h.s. of (8), i.e. b, c are unique functions of the number n_f of massless quarks

$$b = \frac{11N_c - 2n_f}{6}; \quad c = \frac{51N_c - 19n_f}{11N_c - 4n_f}, \quad (9)$$

but all the higher order ones are *completely arbitrary*. Once they are given and some initial condition on a is specified, (8) can be solved. The way of specifying the boundary condition is ambiguous, but its choice is a matter of convention only. One way of doing this is via the scale parameter $\hat{\Lambda}$ introduced in the following implicit equation for the solution of (8) [2]:

$$b \ln \frac{\mu}{\hat{\Lambda}} = \frac{1}{a} + c \ln \frac{ca}{1+ca} + \int_0^a dx \left[-\frac{1}{x^2 B^{(n)}(x)} + \frac{1}{x^2(1+cx)} \right], \quad (10)$$

¹In view of the application to Γ_h we restrict our considerations to quantities depending on a single external momentum Q .

where

$$B^{(n)}(x) \equiv (1 + cx + c_2x^2 + \dots + c_{n-1}x^{n-1}). \quad (11)$$

Note that as the integral on the r.h.s. of (10) behaves like $\mathcal{O}(\alpha_s)$ the higher order coefficients $c_k; k \geq 2$ have no influence on the value of $\tilde{\Lambda}$. Note also that the parameter $\tilde{\Lambda}$ introduced in (10) differs from the Λ used in most phenomenological analyses by a factor close to unity: $\Lambda = \tilde{\Lambda} (2c/b)^{c/b}$. At the next-to-leading order (NLO) – i.e., keeping only the first two terms in (10) – the solution of (10) is often approximated by the first two terms of its expansion in powers of inverse logarithms $\ln(\mu/\Lambda)$:

$$a(\mu/\Lambda) = \frac{1}{b \ln(\mu/\Lambda)} - \frac{c}{b^2} \frac{\ln(\ln(\mu^2/\Lambda^2))}{\ln^2(\mu/\Lambda)} + \dots \quad (12)$$

The dependence of the couplant a on the parameters $c_i; i \geq 2$ is determined by equations similar to (8) [2]:

$$\frac{da(\mu, c_i)}{dc_i} \equiv \beta_i = -\beta(a) \int_0^a \frac{bx^{i+2}}{(\beta(x))^2} dx, \quad (13)$$

which are uniquely determined by the basic β -function in (8) and thus introduce no additional ambiguity.

It is obvious that a unique definition of $a(\mu)$ at some μ requires, as well as the specification of the coefficients $c_i; i \geq 2$, the specification of the boundary condition, – i.e., for instance, the value of $\tilde{\Lambda}$. It is convenient to introduce the concept of the *renormalization convention* (RC), which is associated with a fully defined solution of (8): $\text{RC} \equiv \{\tilde{\Lambda}, c_i; i \geq 2\}$. As, however, μ always enters this solution in the ratio $\mu/\tilde{\Lambda}$, we can either:

- select one of the solutions to (8), which we call referential renormalization convention (RRC) and vary μ only or
- fix μ by identifying it with some external momentum – for instance Q – and vary the solution of (8), i.e., for fixed coefficients c_i the value of Λ instead.

Both these options are completely equivalent and it is merely a matter of taste as to which one to use. We prefer the former. To vary both simultaneously is legal, but obviously redundant.

As the choice of the RRC is a matter of convention only, we cannot associate any physical meaning to the scale μ itself. It serves to label the RS, but only in a given RRC. In two different RRCs the same μ may correspond to different values of the couplant a as well as the coefficients r_k . We emphasize this point as in many papers the RS is chosen by identifying μ with some ‘natural’ physical scale of the process, such as the external momentum Q . Although such a natural scale can usually be identified, its mere existence does not help fix the arbitrary scale μ , as to get a unique RS, the RCC also has to be specified. This is usually tacitly assumed to be the $\overline{\text{MS}}$, but there is no theoretical argument for this choice, except that in this RRC the coefficients r_k are often small. If, however, the magnitude of the coefficients of the perturbative series for physical quantities would be the criterion, we would be naturally drawn to the effective charges approach,

described below, where they actually vanish. In other words, because the choice of the $\overline{\text{MS}}$ as the RRC is merely a convention, there is no reason to set $\mu = Q$.

The above relation (10) allows the expression of $\mu/\tilde{\Lambda}$ in terms of a and c_i and thus the labelling the RS by means of the set of parameters $a, c_i; i \geq 2$. Using this way of labelling the RS is very convenient as there is then no need to introduce the RRC and also no possibility of referring to the ‘natural’ scale to fix the RS.

In the NNLO order – i.e., taking into account also the first nonunique coefficient c_2 – we have the equation

$$b \ln \frac{\mu}{\tilde{\Lambda}} = \frac{1}{a} + c \ln \frac{ca}{\sqrt{1+ca+c_2a^2}} + f(a, c_2), \quad (14)$$

where

$$\begin{aligned} f(a, c_2) &= \frac{2c_2 - c^2}{d} \left(\arctan \frac{2c_2a + c}{d} - \arctan \frac{c}{d} \right); \quad d \equiv \sqrt{4c_2 - c^2}; \quad 4c_2 > c^2 \\ &= \frac{2c_2 - c^2}{d} \left(\ln \left| \frac{2c_2a + c - d}{2c_2a + c + d} \right| - \ln \left| \frac{c - d}{c + d} \right| \right); \quad d \equiv \sqrt{c^2 - 4c_2}; \quad 4c_2 < c^2. \end{aligned} \quad (15)$$

Its solution depends on the value of c_2 . We distinguish three different cases:

- $c_2 = 0$ (resp. $c_i = 0, i \geq 2$), defining the so called ‘t Hooft RC [3]
- $c_2 > 0$, when $\beta(a) < 0$ is monotonously decreasing function of a and the situation is therefore qualitatively the same as for $c_2 = 0$
- $c_2 < 0$, when $\beta(a)$ has the *infrared fixed point* at $a^*(c_2)$, given by the equation $\beta[a^*(c_2)] = 0$. The corresponding solution of (8) then approaches *finite* value at $\mu = 0$ and consequently

$$\lim_{Q \rightarrow 0} r^{(3)}(Q) = a^*(c_2) \left(1 + r_1(\mu = Q) a^*(c_2) + r_2(c_2, \mu = Q) a^{*2}(c_2) + \dots \right) \quad (16)$$

has a finite *infrared limit* at the NNLO. This case is discussed in detail in Refs. [4, 5].

Note that the possibility of an infrared stable limit of finite order approximants, which starts at the NNLO, does not have to survive the incorporation of still higher order corrections and its physical relevance is therefore questionable.

While the explicit dependence of the couplant on c_i is given in (14) and (15), the dependence of the coefficients r_k on them is determined by the requirements of internal consistency of the perturbation theory. They imply that any finite order approximant

$$r^{(N)}(Q) \equiv \sum_{k=0}^{N-1} r_k a^{k+1} = \mathcal{F}(\mu, c_i, \rho_i; i \leq N-1), \quad (17)$$

must satisfy the following consistency conditions:

$$\frac{dr^{(N)}}{d \ln \mu} = \mathcal{O}(a^{N+1}), \quad \frac{dr^{(N)}}{dc_i} = \mathcal{O}(a^{N+1}). \quad (18)$$

Iterating these equations we find:

$$\begin{aligned} r_1(Q/\mu) &= b \ln \frac{\mu}{Q} + r_1(\mu = Q) = b \ln \frac{\mu}{\tilde{\Lambda}} - \rho(Q/\tilde{\Lambda}) \\ r_2(Q/\mu, c_2) &= \rho_2 - c_2 + r_1^2 + cr_1, \end{aligned} \quad (19)$$

and similarly for still higher orders. In the above relations the quantities ρ, ρ_2 etc., are RG invariants – i.e., contrary to the coefficients r_k , they are independent of the choice of the RS. Note that all the dependence of the perturbative approximants on Q comes exclusively through the invariant $\rho(Q/\Lambda)$, which can be written as

$$\rho = b \ln(Q/\tilde{\Lambda}_{\text{RRC}}) - r_1(\mu = Q, \text{RRC}), \quad (20)$$

where the apparent dependence on the chosen RRC actually cancels between the two terms in (20).

A nontrivial part of any perturbative calculation boils down to the evaluation of these invariants, the rest being essentially a straightforward exploitation of the RG considerations based on (18). Substituting for the term $b \ln(\mu/\Lambda)$ in r_1 the expression (10), using (19) and inserting the resulting r_k into (17), any finite order approximant $r^{(N)}(Q)$ can be expressed as an explicit function of the parameters specifying the RS, i.e., $a, c_i; i \geq 2$, and the invariants ρ_i :

$$r^{(N)}(Q) = f(\rho_j, j < N - 1; a, c_i, i \leq N - 1). \quad (21)$$

In this representation the RS dependence of NLO and NNLO approximants is quantitatively described by one- and two-dimensional manifolds, respectively, and the problem of choosing the RS is equivalent to selecting one particular point on these manifolds. Considered as a geometrical exercise we identify certain special points on these manifolds, corresponding to stationary points, where the variation of the approximants with respect to the free parameters vanishes locally.

In the next subsection we shall briefly describe some of the criteria for choosing the RS, which will define the set of RS for which we shall later estimate the theoretical uncertainty of perturbative calculations of the quantities of interest. We shall discuss in some more detail the approaches described in subsections 2.5 and 2.6, as there have recently been some new developments in them.

2.2 Fixed RS calculations

Because of the computational simplicity and explicit gauge invariance, all the multiloop calculations are nowadays done using the dimensional regularization technique. Within this technique the $\overline{\text{MS}}$ renormalization prescription² is often preferred on the grounds that it absorbs in the definition of the renormalized couplant the terms proportional to $\ln 4\pi - \gamma_E$, which are considered to be artefacts of the dimensional regularization technique. In our way of labelling the RS, $\overline{\text{MS}}$ corresponds to definite values of all the coefficients r_k, c_k and a fixed, but numerically undetermined, value of a , which must be extracted

²By ‘prescription’ we mean the specification of the scale μ (by identifying it with some natural scale Q) as well as of finite parts of all counterterms necessary to cancel the UV divergencies. Specifying the prescription implies the specification of the RS in the above-defined sense, but not vice versa.

from comparison with experimental data. This choice of the RS is very commonly used in phenomenological analyses, but there is no obvious reason why it should be preferred to, for instance, the MOM-like RS or any of the choices discussed in the following subsections. In geometrical terms this is reflected in the fact that the corresponding point on the hypersurfaces defined in (21) occupies no special position.

2.3 Principle of Minimal sensitivity (PMS)

In this approach, suggested in Ref. [2], the RS is fixed by demanding that

$$\frac{dr^{(N)}}{da} = \frac{dr^{(N)}}{dc_i} = 0, \quad (22)$$

i.e., the N -th order partial sum has locally the property that the full expansion must satisfy globally. Though there is in general no guarantee that such a stationary point is unique or exists at all, in practical applications to lowest order QCD quantities it works. At the NLO, when only a labels the RS, (22) reduces to

$$2 - 2\rho a + 2ca \ln \frac{ca}{1+ca} + ca \left(\frac{ca}{1+ca} \right) = 0, \quad (23)$$

and its solution has the form $a_{\text{PMS}} = (1/\rho)[1 + \mathcal{O}(ca_{\text{PMS}})]$.

At the NNLO we have two coupled equations for derivatives of $r^{(2)}(a, c_2)$ with respect to a and c_2 , which must be solved numerically. For the quantity (7) such a stationary point exists for any ρ if $\rho_2 < 0$ and for $\rho > \rho_{\min}(\rho_2)$ if $\rho_2 > 0$ [4].

Note that, contrary to the fixed RS approach, the PMS selects the RS which depends on the type and kinematics of the process under study. The same holds for the methods discussed in the next three subsections.

2.4 The method of effective charges (ECH)

The basic idea of this approach [6] is to choose the RS in such a way that the relation between the physical quantity and the couplant is the simplest possible one. For the quantity (7) it means:

$$r(Q) = a_{\text{ECH}}. \quad (24)$$

In this approach there is no problem with the convergence of the perturbation expansion (7) itself, but it reappears in the perturbation expansion of the corresponding β -function (see below).

The conditions under which the parameters a , c_i , or μ , c_i , can be chosen in such a way that (24) holds can be read directly off the consistency conditions (18). At the NLO, (24) implies the following equation for a^{ECH}

$$\frac{1}{a} + ca \ln \frac{ca}{1+ca} = \rho, \quad (25)$$

which has a solution $a_{\text{ECH}} = (1/\rho)(1 + \mathcal{O}(ca_{\text{ECH}}))$, differing from a^{PMS} merely by the term of the order $\mathcal{O}(ca_{\text{ECH}})$. At the NLO the values of a_{ECH} thus correspond to intersections

of the curves defined as

$$r^{(2)}(a, c_2) = a \left(2 - \rho a + ca \ln \frac{ca}{1 + ca} \right), \quad (26)$$

with the straight line $r^{(2)} = a$. For $\rho > 0$ there is always just one such intersection in the physically relevant range $a > 0$, while for $\rho < 0$ there is none in this range.

At the NNLO the situation is more complicated, as the condition (24) does not by itself determine uniquely a_{ECH} , but merely implies the equation

$$r_1(a) + r_2(a, c_2)a = 0, \quad (27)$$

which has, depending on the value of c_2 , either no solution, or one or two solutions, giving *different* a_{ECH} . Going to still higher orders the ambiguity of this approach grows even further as new free parameters, c_i , crop up. In [6] this ambiguity is avoided by demanding that each of the coefficients r_i vanishes individually. Assuming this restricted version of the ECH method – i.e., demanding $r_i = 0, i \geq 1$ – we get the following expression for the associated β -function:

$$\frac{da_{\text{ECH}}}{d \ln \mu} \equiv \beta_{\text{ECH}}(a) = -ba_{\text{ECH}}^2 \left[1 + \rho_1 a_{\text{ECH}} + \rho_2 a_{\text{ECH}}^2 + \dots \right], \quad (28)$$

where $\rho_1 \equiv c$. The coefficients $c_{\text{ECH},i}$ of the ECH β -function β_{ECH} thus coincide with the RG invariants ρ_i , introduced in (19). To express a_{ECH} as a function of the external momentum Q , it is convenient to write it as a solution of the equation

$$\frac{1}{a_{\text{ECH}}} + c \ln \frac{ca_{\text{ECH}}}{1 + ca_{\text{ECH}}} = b \ln \frac{Q}{\Lambda_{\text{ECH}}}, \quad (29)$$

where Λ_{ECH} defines the ‘effective’ Λ parameter, associated with the quantity under study. It is related to Λ_{RS} in any fixed RS simply as

$$\Lambda_{\text{ECH}} = \Lambda_{\text{RS}} \exp(r_1(\mu = Q, \text{RS})/b). \quad (30)$$

As the ECH approach seems to offer a very simple and natural ‘solution’ to the RS problem one might naturally ask: where has all the ambiguity discussed in subsection 2.1 actually gone? In fact it has not disappeared entirely and reemerges, as discussed in Ref. [7], in a somewhat disguised form, even within the ECH approach.

2.5 The method of Brodsky, Lepage and MacKenzie

This method [8] borrows its basic idea from QED, where the renormalized electric charge is fully given by the vacuum polarization due to charged fermion–antifermion pairs. In QCD the authors of this method suggest fixing the scale μ with the requirement that all the effects of quark pairs be absorbed in the definition of the renormalized couplant itself, leaving nothing in the expansion coefficients. In the case of the quantity (7) and up to the NNLO,

$$r(Q) = a(\mu, \text{RRC}) \left(1 + \left[r_{10} \left(\frac{\mu}{Q}, \text{RRC} \right) + n_f r_{11} \left(\frac{\mu}{Q}, \text{RRC} \right) \right] a(\mu, \text{RRC}) \right), \quad (31)$$

where we have now written the n_f dependence of the coefficients r_k explicitly, it amounts to the requirement that μ be chosen in such a way that $r_{11}(\mu/Q, \text{RRC}) = 0$. The problem with this ‘scale-setting’ method is that the resulting scale as well as r^{BLM} depend on the choice of the RRC! This is due to the fact that for a given μ the separation of the coefficient r_1 into the two parts $A + n_f B$ is *not unique*, but depends on the RRC used. This problem exists in principle QED as well, but there the quark loop effects can be rather unambiguously absorbed in the renormalized electric charge via the MOM RRC, which for massless quarks gives the same B as the MS-like ones. This is no longer true in QCD, where various types of MOM-like RRC in general give different values of B , different again from that of $\overline{\text{MS}}$ -like one [9].

As emphasized in the general discussion above, fixing the scale without also simultaneously fixing the RRC does not, however, determine the RS, because the choice of the RRC is equally important as that of the scale μ . The resulting ambiguity of the BLM approach, pointed out a long time ago [9], has not yet been satisfactorily resolved. In practical applications one usually starts from the $\overline{\text{MS}}$ RRC.

It is claimed in Ref. [8] that the BLM-improved expressions for the physical quantities have small NLO coefficients. However, as shown in Ref. [10], this is not necessarily the case when the BLM approach is generalized to higher orders. Let us first recall the main steps of the generalization suggested in Ref. [10].

Within the class of the so called ‘regular’ RC the n_f dependence of the expansion as well as β -function coefficients is polynomial in n_f :

$$\begin{aligned}
r_1 &= r_{10} + r_{11}n_f \\
r_2 &= r_{20} + r_{21}n_f + r_{22}n_f^2 \\
\beta_0 &\equiv b = b_{00} + b_{01}n_f \\
\beta_1 &\equiv bc = \beta_{10} + \beta_{11}n_f \\
\beta_2 &\equiv bc_2 = \beta_{20} + \beta_{21}n_f + \beta_{22}n_f^2 + \beta_{23}n_f^3 \\
\tilde{\beta}_2 &\equiv b\rho_2 = \tilde{\beta}_{20} + \tilde{\beta}_{21}n_f + \tilde{\beta}_{22}n_f^2 + \tilde{\beta}_{23}n_f^3.
\end{aligned} \tag{32}$$

Note that the scheme-invariant coefficient $\tilde{\beta}_2$ contains the n_f^3 term as observed in Ref. [11].

The generalization of the BLM approach suggested in [10] assumes that the chosen scale μ is determined by the following perturbative expansion:

$$\mu^2 = \mu_{\text{BLM}}^2 \left(1 + \gamma_1(n_f)a(\mu_{\text{BLM}}) + \dots \right), \tag{33}$$

where μ_{BLM}^2 is given in [8] and $\gamma_1 = \gamma_{10} + \gamma_{11}n_f$. The parameters γ_{10} and γ_{11} are process dependent and can be determined from the following system of equations³

$$\begin{aligned}
\tilde{\beta}_{23} - \beta_{23} &= -2\beta_{01}^2\gamma_{11} \\
\tilde{\beta}_{22} - \beta_{22} &= -2\beta_{01}^2\gamma_{10} - 4\beta_{00}\beta_{11}\gamma_{11}
\end{aligned}$$

³Note the factor-of-two difference between our definition (8) of the β -function and that used in Ref. [10].

$$\begin{aligned}
\tilde{\beta}_{21} - \beta_{21} &= \beta_{01} \left(r_2^* - r_1^{*2} \right) - \beta_{11} r_1^* - 4\beta_{00}\beta_{01}\gamma_{10} - 2\beta_{00}^2\gamma_{11}^2 \\
\tilde{\beta}_{20} - \beta_{20} &= \beta_{00} \left(r_2^* - r_1^{*2} \right) - \beta_{10} r_1^* - 2\beta_{00}^2\gamma_{10},
\end{aligned} \tag{34}$$

which follows from the general expression for the scheme invariant $\tilde{\beta}_2$:

$$\tilde{\beta}_2 = \beta_2 + b r_2 - \beta_1 r_1 - b r_1^2. \tag{35}$$

In the above equations, r_1^* and r_2^* are the n_f -independent coefficients in the generalized BLM procedure. We have already mentioned that in practice the BLM approach is applied to the initial series with the coefficients defined in the $\overline{\text{MS}}$ -scheme. Therefore, it is necessary to put $\beta_{23} = 0$. Now consider as an example perturbation expansion for the familiar quantity:

$$R(s) \equiv \frac{\sigma(e^+e^- \rightarrow \text{hadrons})}{\sigma(e^+e^- \rightarrow \mu^+\mu^-)} = \left(3 \sum_{i=1}^{n_f} Q_i^2 \right) \left[1 + \sum_{k=0}^{\infty} r_k a^{k+1} \right]. \tag{36}$$

Applying the above generalization to (36) we get [10]

$$\mu_{\text{BLM}}^2 = \mu_{\overline{\text{MS}}}^2 \exp(0.69), \quad \gamma_{01} = 0.11, \quad \gamma_{11} \approx 3, \tag{37}$$

which implies

$$R(s) = \left(3 \sum_{i=1}^{n_f} Q_i^2 \right) \left[1 + a_* + 0.08a_*^2 - 23.3a_*^3 \right] - \left(\sum_{i=1}^{n_f} Q_i \right)^2 1.24a_*^3, \tag{38}$$

where

$$a_* = a \left(\mu_{\text{BLM}}^2 (1 + \gamma_1(n_f) a(\mu_{\text{BLM}}^2)) \right). \tag{39}$$

Notice that the coefficient of the NNLO correction is, indeed, not small. Therefore it is not true, as conjectured in Ref. [8], that the BLM-improved perturbative series have in general significantly smaller coefficients than the expansions in the $\overline{\text{MS}}$.

2.6 RS invariant perturbation theory

The basic problem of RS dependence can be traced back to the fact that the expansion parameter, the renormalized couplant a , is not a physical quantity, but rather an intermediate variable, allowing us to correlate different physical quantities. As such, it is inevitably ambiguous. This problem can be circumvented – at least in part – by expressing one physical quantity directly as power expansion in terms of the other. Consider, for instance, two physical quantities admitting the following perturbation expansions in some RS⁴

$$\begin{aligned}
R^{(1)} &= a(\text{RS}) \left(1 + r_1^{(1)}(\text{RS}) a(\text{RS}) + \dots \right) \\
R^{(2)} &= a(\text{RS}) \left(1 + r_1^{(2)}(\text{RS}) a(\text{RS}) + \dots \right)
\end{aligned} \tag{40}$$

⁴There is no problem generalizing this analysis to the case of different powers of the leading terms.

Expressing $a(\text{RS})$ from the first in terms of $R^{(1)}$ and substituting into the second equation we get

$$R^{(2)} = R^{(1)} \left(1 + \Delta^{(2,1)} R^{(1)} + \dots \right), \quad (41)$$

where $\Delta^{(2,1)} = r_1^{(2)}(\text{RS}) - r_1^{(1)}(\text{RS})$, as well as all the other coefficients $\Delta^{(2,j)}$, $j \geq 2$ of this expansion, *are unique*. This kind of expansion has already been discussed within the so-called ‘scheme invariant perturbation theory’ in Ref. [12] and recently resurected within the so called ‘commensurate scale relations’ in [13]. The essence, however, remains the same.

As a special and interesting example of such a relation, consider the one between the derivative of (7) with respect to the external momentum Q and the quantity $r(Q)$ itself. It is straightforward exercise to show that this relation reads:

$$\frac{dr(Q)}{d \ln Q} = -b[r(Q)]^2 \left(1 + cr(Q) + \rho_2[r(Q)]^2 \dots \right) = \beta_{\text{ECH}}(r(Q)), \quad (42)$$

where the r.h.s. is nothing else than the ‘effective’ β -function introduced above, evaluated at $r(Q)$!

In (41) as well as in (42) there is no trace of any RS ambiguity. It is nice to be able to show explicitly, as is done in Refs. [12–14], that all the coefficients in these expansions are, indeed, RS invariants, but it cannot be otherwise, as they relate two physical variables and there is no way their eventual dependence on the RS could be cancelled. Perturbation theory serves here merely as an intermediate, but vital, tool for evaluating coefficients such as $\Delta^{(2,j)}$ and ρ_i .

If relations such as (41) or (42) are truly unique, do they not solve the whole RS-dependence problem? The answer depends on what we expect from the perturbation theory. If we are interested merely in relating pairs of physical quantities admitting purely perturbative expansions the answer is positive. If, however, we ask the question: what is, on the basis of analyses of available experimental data, the QCD prediction for, say, the Z^0 width, then the answer is definitely negative. The point is that in predicting the value of Γ_h from the relations between this quantity and some other physical quantity R , we find that the resulting predictions *depend on the choice of the quantity R*! What has been thrown out the door in the form of the RS ambiguity, comes back through the window as the ‘initial condition’ ambiguity [15]. Moreover, this new one is even more difficult to handle than the original one!

We therefore believe that the better way of incorporating the results of QCD analyses of many different physical quantities measured in different kinematical ranges is to introduce some intermediate, no-nunique and thus *unphysical*, variable, which can then be used for QCD predictions of other physical quantities. The renormalized couplant serves just this purpose.

3 Quark mass thresholds in the running α_s

The proper treatment of quark mass effects in the QCD running coupling constant α_s has so far not been in the forefront of interest of theorists and phenomenologists. This

is now changing. Although the quark mass effects are not large, steady improvement in the precision of experimental data, coming in particular from a new generation of experiments at CERN and Fermilab, combined with significant progress in higher order QCD calculations, has led to a renewed interest in quantitative aspects of these effects [16, 17, 18]. There are two basic reasons for this, both of which are relevant to the subject of this article.

The first concerns the exploitation of the complete NNLO QCD calculations that have recently become available for quantities such as (36) [19] or Γ_h [20, 21] and which exist basically for massless quarks only. The NNLO corrections are tiny effects and to include them makes sense only if they are large compared to errors resulting from the approximate treatment of the quark mass thresholds in massless QCD. To quantify the importance of the NNLO correction to the couplant α_s , consider the difference between the values of $\alpha_s(\overline{\text{MS}}, M_Z)$ in the NLO and NNLO approximations, assuming five massless quarks and taking, as an example, $\Lambda_{\overline{\text{MS}}}^{(5)} = 0.2$ GeV. At the NLO the couplant $a \equiv \alpha_s/\pi$ is given as a solution to Equation (14) for $c_2 = 0$ and we get $a^{\text{NLO}}(\overline{\text{MS}}, M_Z) = 0.03742$. At the NNLO and in $\overline{\text{MS}}$ RS, where $c_2(\overline{\text{MS}}, n_f = 5) = 1.475$, we find $a^{\text{NNLO}}(\overline{\text{MS}}, M_Z) = 0.03665$. The relative difference between these two approximations,

$$\frac{a^{\text{NLO}} - a^{\text{NNLO}}}{a^{\text{NLO}}} \doteq 0.02, \quad (43)$$

thus amounts to about 2%. The NNLO correction should therefore be included only if the neglected effects can be expected to be smaller than this number. However, as we shall see, quark mass threshold effects can in some circumstances be of just this magnitude!⁵

The second reason is related to the problem of comparing the values of α_s , determined from different quantities characterized by vastly different momentum scales. As recently emphasized in an extensive review of α_s determinations [22], there is a small, but non-negligible discrepancy between the value of $\alpha_s(\overline{\text{MS}}, M_Z)$ obtained by extrapolation from some of the low energy quantities, and $\alpha_s(\overline{\text{MS}}, M_Z)$ determined directly at the scale M_Z at LEP – the latter giving the value higher by about 5–10%. Simultaneously, it has been noted in ref. [22] that there is an exception to this behaviour in the case of the ratio R_τ , which, when extrapolated from m_τ to M_Z , gives values of α_s close to those measured directly at LEP (0.120 ± 0.005 [23]). The physical relevance of the discrepancy between the low energy extrapolations and direct measurements of α_s at LEP has very recently been emphasized in Ref. [24]. In particular, its author argues that the extrapolation of $\alpha_s(m_\tau)$ to $\alpha_s(M_Z)$ is unreliable due to limited control of the power corrections. The question of estimating the theoretical uncertainty in the extraction of $\alpha_s(m_\tau)$ from data on R_τ is also discussed in ref. [25] As shown in [18], a part of this overestimate of the extrapolated value of $\alpha_s(M_Z)$ pointed out in [24] may in fact be due to the approximate treatment of the c and b quark thresholds.

We shall now analyze the quantitative consequences of the exact treatment of quark mass thresholds at the LO and formulate the conventional matching procedure [26] for massless quarks in such a way that its results are so close to those which are exact that

⁵ In general, as the magnitude of higher order corrections to α_s depends on the renormalization scheme employed, so does also the estimate (43). However, if defined as the relative difference between the NLO and NNLO approximations, this dependence is not strong (see the concluding paragraph of Section 4).

the available NNLO calculation can be consistently included. We shall describe in detail the approximation in which the u, d and s quarks are considered massless while the c, b and t quarks remain massive.

As complete multiloop calculations with massive quarks are very complicated and available only at the leading order, all higher order phenomenological analyses use the calculations with a fixed effective number n_f of massless quarks, depending on the characteristic scale of the quantity. For relating two regions of different effective numbers of massless quarks the approximate matching procedure developed in Ref. [26] is commonly used. It should be emphasized that this procedure concerns only those mass effects that can be absorbed in the renormalized couplant. At higher orders there are, however, mass effects that remain in the expansion coefficients even after the effects of heavy quarks have been absorbed in a suitably defined running couplant.

In QCD with massive quarks the renormalization group equation for the couplant $a(\mu)$ formally looks the same as in massless QCD. The only, but important, difference concerns the two lowest order β -function coefficients, $b, \beta_1 = bc$, which are no longer unique as in massless QCD, but may depend on the scale μ . While in the class of $\overline{\text{MS}}$ -like renormalization conventions $b = 11/2 - n_f/3$, exactly as in massless QCD, in MOM-like ones it becomes a nontrivial function of the scale μ [27]:

$$b(\mu/m_i) = \frac{11}{2} - \frac{1}{3} \sum_i h_i(x_i), \quad x_i \equiv \frac{\mu}{m_i}, \quad (44)$$

where the sum runs over all the quarks considered, m_i are the corresponding renormalized quark masses⁶ and the threshold function $h(x)$ is given as Ref. [27]. The shape of the function $h(x)$ is actually not quite unique and depends on the vertex chosen for the definition of the renormalized couplant. This fact was first noted in Ref. [28] and subsequently explained in Ref. [29]. The form of $h(x)$ used below corresponds to quark-gluon-quark vertex with massless quarks, using any momentum configuration and any invariant decomposition in MOM-like RS [29]. It is appropriate for most of the extrapolations from low energy quantities to LEP energy range. The same form is valid for the ghost-gluon-ghost vertex. The three gluon vertex gives somewhat different form of $h(x)$, though its behaviour for small and large x is the same. According to [27]:

$$h(x) \equiv 6x^2 \int_0^1 dz \frac{z^2(1-z)^2}{1+x^2z(1-z)} = 1 - \frac{6}{x^2} + \frac{12}{x^3\sqrt{4+x^2}} \ln \frac{\sqrt{4+x^2}+x}{\sqrt{4+x^2}-x} \doteq \frac{x^2}{5+x^2}. \quad (45)$$

The last, approximate, equality is a very accurate approximation of the exact form of $h(x)$ in the whole range $x \in (0, \infty)$. This allows a simple treatment of the quark mass thresholds at the LO. There is, unfortunately, no analogous calculation of the next β -function coefficient, bc , for massive quarks. This is one of the reasons why most of the phenomenological analyses use the so called ‘step’ approximation, in which at any value of μ one works with a finite effective number of massless quarks, which changes discontinuously at some matching points μ_i . Consequently, $b(n_f)$ effectively becomes a function of μ , discontinuous at these matching points, as shown in Fig.1a.

⁶For the purposes of this discussion quark masses can be regarded as constants. In numerical estimates they are identified with the running masses at the scale M_Z .

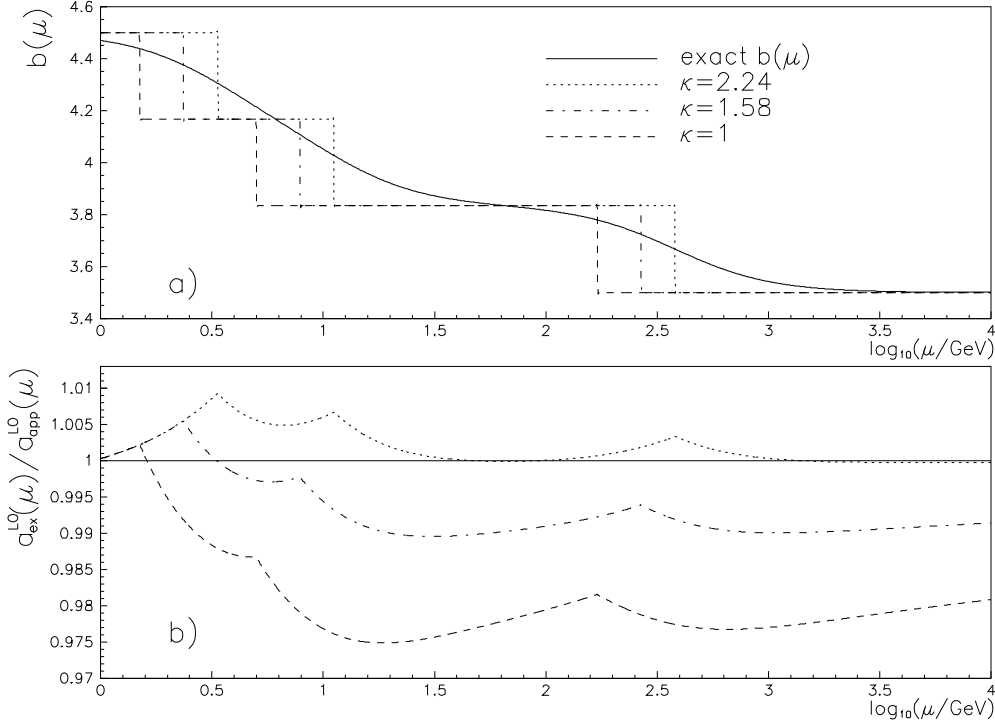


Figure 1: a) $b(\mu/m_i)$ together with three step approximations, corresponding to matching at the points $\mu_i = \kappa m_i$; $i = c, b, t$ with $\kappa = 1, 1.58, 2.24$; b) the ratio R_a for the same three approximations, made to coincide at $\mu_0 = 1$ GeV.

The matching points are assumed to be proportional to the masses of the corresponding quarks, $\mu_i \equiv \kappa m_i$. In principle, a different quark threshold could be associated with a different κ , but for simplicity's sake we take them equal. The free parameter κ , allowing for the variation of the proportionality factor, turns out to be quite important for the accuracy of the step approximation. At the LO the matching procedure then consists of the following relations at the matching points μ_i (the numbers in the superscript define the corresponding effective number of massless quarks)⁷:

$$a_{\text{app}}^{\text{LO},3}(\kappa m_c/\Lambda^{(3)}) = a_{\text{app}}^{\text{LO},4}(\kappa m_c/\Lambda^{(4)}) \Rightarrow \Lambda^{(4)} = \Lambda^{(3)} \left(\frac{\Lambda^{(3)}}{\kappa m_c} \right)^{1/3b(4)} \quad (46)$$

$$a_{\text{app}}^{\text{LO},4}(\kappa m_b/\Lambda^{(4)}) = a_{\text{app}}^{\text{LO},5}(\kappa m_b/\Lambda^{(5)}) \Rightarrow \Lambda^{(5)} = \Lambda^{(4)} \left(\frac{\Lambda^{(4)}}{\kappa m_b} \right)^{1/3b(5)} \quad (47)$$

$$a_{\text{app}}^{\text{LO},5}(\kappa m_t/\Lambda^{(5)}) = a_{\text{app}}^{\text{LO},6}(\kappa m_t/\Lambda^{(6)}) \Rightarrow \Lambda^{(6)} = \Lambda^{(5)} \left(\frac{\Lambda^{(5)}}{\kappa m_t} \right)^{1/3b(6)}. \quad (48)$$

Note that each of the intervals of fixed n_f is associated with a different value of the Λ -parameter, $\Lambda^{(n_f)}$. The resulting dependence of $a(\mu/m_i)$ on μ is thus continuous at each of the matching points, but its derivatives at these points are discontinuous, reflecting

⁷The parameter Λ appearing in this as well as the other formulae in this section is the leading order Λ parameter, Λ^{LO} , which cannot be associated with any well-defined RS. As there is no danger of confusion, we shall drop the superscript 'LO' for the remainder of this section.

the discontinuity of the step approximations to $b(\mu/m_i)$. This procedure can easily be extended to any finite order. Let us point out that the more sophisticated procedure for matching the couplants corresponding to different effective n_f developed in Ref. [30] coincides in the LO with the above relations (48–50). To estimate the errors in α_s resulting from the above-defined approximate treatment of quark thresholds we merely need solve the LO equation with exact explicit mass dependence as given in (44):

$$\frac{da(\mu)}{d \ln \mu} = -a^2 \left(\frac{11}{2} - \frac{1}{3} \sum_{i=1}^6 h(x_i) \right). \quad (49)$$

For our purposes the approximation $h(x) \doteq x^2/(5 + x^2)$ is entirely adequate and yields

$$a(\mu) = \frac{1}{\left(\frac{11}{2} - \frac{3}{3} \right) \ln \frac{\mu}{\Lambda^{(3)}} - \frac{1}{3} \sum_{i=c,b,t} \ln \frac{\sqrt{\mu^2 + 5m_i^2}}{\sqrt{(\Lambda^{(3)})^2 + 5m_i^2}}}, \quad (50)$$

where the fraction $\frac{3}{3}$ comes from the sum over the three massless quarks u, d and s and $\Lambda^{(3)}$ is the corresponding Λ -parameter appropriate to three massless quarks. For the heavy quarks c, b and t we take in the following $m_c = 1.5$ GeV, $m_b = 5$ GeV, $m_t = 170$ GeV. The distinction between the ‘light’ and ‘heavy’ quarks is given by the relative magnitude of m_i and Λ , the latter being defined by the condition $5m_i^2 \gg \Lambda$. For the above values of m_c, m_b and m_t this condition is very well satisfied. Consequently, for $\mu \ll m_i, i = c, b, t$ (50) approaches smoothly a^{LO} for $n_f=3$, while for $\mu \gg m_i$, and neglecting $\Lambda^{(3)}$ with respect to $5m_i^2$, it goes to

$$a(\mu) = \frac{1}{b(6) \ln \frac{\mu}{\Lambda^{(3)}} + \frac{1}{3} \ln \left(\frac{\sqrt{5}m_c}{\Lambda^{(3)}} \frac{\sqrt{5}m_b}{\Lambda^{(3)}} \frac{\sqrt{5}m_t}{\Lambda^{(3)}} \right)} = \frac{1}{b(6) \ln \frac{\mu}{\Lambda^{(6)}(\sqrt{5})}}, \quad (51)$$

where the parameter $\Lambda^{(6)}(\kappa)$ depends in general on κ and

$$\Lambda^{(6)}(\sqrt{5}) \equiv \Lambda^{(3)} \left(\frac{\Lambda^{(3)}}{\sqrt{5}m_c} \frac{\Lambda^{(3)}}{\sqrt{5}m_b} \frac{\Lambda^{(3)}}{\sqrt{5}m_t} \right)^{\frac{1}{3b(6)}} = \left(\frac{1}{\sqrt{5}} \right)^{\frac{1}{b(6)}} \Lambda^{(6)}(1) \quad (52)$$

coincides with $\Lambda^{(6)}$ defined via the subsequent application of the matching relations (48–50) for $\kappa = \sqrt{5} \doteq 2.24$. Even though from the point of view of the matching procedure, κ is not exactly fixed, the value $\kappa = \sqrt{5}$ will be shown to be in a certain sense the best choice. The relation between $\Lambda^{(6)}$ and $\Lambda^{(3)}$ depends nontrivially on κ .

In Fig. 1a, $b(\mu)$ is plotted as a function of μ for the above-mentioned masses of c, b and t quarks, together with its step approximations and corresponding to three different values of $\kappa = 1, \sqrt{5}, \sqrt{5}/2$. There is hardly any sign of the steplike behaviour of the function $h(x)$ in the region of the c and b quark thresholds and only a very unpronounced indication of the plateau between the b and t quark thresholds. The step approximations are poor representations of the exact $h(x)$, primarily due to the rather slow approach of $h(x)$ to unity as $x \rightarrow \infty$. However, there is a marked difference between the three approximations.

While the step approximation with the conventional choice $\kappa = 1$ underestimates the true $h(x)$ in the whole interval displayed, and would do so even when some smoothing were applied, $\kappa = \sqrt{5}$ gives clearly much better approximation as the corresponding curve is intersected by the exact $h(x)$ at about the middle of each step.

In Fig. 1b the μ dependence of the ratio

$$R_a \equiv \frac{a_{ex}^{LO}(\mu)}{a_{app}^{LO}(\mu)}, \quad (53)$$

between the above exact solution (51) and the approximate expressions for the above mentioned values of κ , is plotted assuming $\Lambda^{(3)} = 200$ MeV⁸. As we basically want to compare the results of different extrapolations starting from the same initial μ_0 , $\Lambda^{(3)}$ used in the approximate solutions has been rescaled by the factor 1.004 with respect to $\Lambda^{(3)}$ in (50), thereby guaranteeing that all expressions coincide at $\mu_0 = 1$ GeV. Any deviation from unity in Fig. 1b is then entirely the effect of an approximate treatment of the heavy quark thresholds. Figure 1 contains several simple messages.

The approximate solutions based on the matching procedure defined in (48–50) are generally much better immediately *below* the matching point than above it, and worst at about $5m_{\text{match}}$. This reflects the fact that the function $h(x)$ vanishes fast (like x^2) at zero but approaches unity for $x \rightarrow \infty$ only very slowly. Moreover, in the M_Z range the effect of the c quark threshold is essentially the same as that of the b quark and both are much more important than that of the top quark, although $M_Z/m_c \approx 60$, $M_Z/m_b \approx 18$, while $M_Z/m_t \approx 1/2$!

The effect of varying κ is quite important, in particular with respect to the c and b quark thresholds. In general, $\kappa > 1$ improves the approximation above, but worsens it immediately below the matching point it. The choice $\kappa = \sqrt{5}$, suggested by the asymptotic behaviour of (51), is clearly superior in practically the whole displayed interval $\mu \in (1, 10^4)$ GeV and leads to an excellent (on the level of 0.1%) agreement with the exact solution in this interval. On the contrary, the conventional choice $\kappa = 1$ leads to a much larger deviation from the exact result, which exceeds 2% in most of this region. This discrepancy is of the same magnitude as the effects of NNLO corrections to the couplant itself. It thus turns out that the effect of an exact treatment of the quark mass thresholds for the extrapolation of α_s from the scales around $\mu \approx 2$ GeV up to $\mu = M_Z$ is as important as that of the NNLO correction to α_s and must therefore be taken into account whenever the latter is considered and compared with α_s determined at these vastly different scales.

On the other hand, the preceding discussion tells us little about the accuracy of the approximation of five massless quarks directly at the scale M_Z , for instance when calculating Γ_h . This question will be addressed in section 5.

The analysis of quark mass effects in α_s presented above strictly speaking holds only for the LO. Nevertheless, as both the mass effects and the higher order perturbative corrections are small effects, it seems reasonable to expect that the conclusions drawn in this section will have more general validity.

⁸ The resulting ratio $R_a(M_Z)$ depends only weakly on $\Lambda^{(3)}$. Note, however, that the current analysis of the LEP data gives the value of $\Lambda^{(3)}$ in the range 500–700 MeV in disagreement with the QCD sum rules analysis [24].

4 Application to Γ_h

We now come to the quantitative estimate of the theoretical uncertainties of perturbative QCD predictions for Γ_h . In the preceding section we discussed the approximation in which α_s is given by an expression corresponding to five massless quarks. In this section we quantify the uncertainties resulting from the RS ambiguity, discussed in Section 2. The nontrivial dependence of Γ_h on m_b and m_t , coming from effects not included in the running couplant corresponding to five massless quarks, is discussed in the next section. Nevertheless in order to avoid unnecessary repetition we include the dependence on the ratio M_Z/m_t already in the formulae quoted below and obtained recently in Refs. [19, 20, 21, 31, 32]. The dependence of the expansion coefficients on the bottom quark mass has extensively been studied in Ref. [33]. We do not write it out here explicitly, as this would further complicate the structure of (54), each of the coefficients in (54) becoming a different function of the ratio m_b/M_Z . At the end of this section we shall merely recall the leading contributions to R_Z coming from m_b/M_Z terms and discuss their numerical importance.

In order to quantify the theoretical uncertainty related to the choice of the RS, we first define the set of ‘allowed’ RS. As emphasized above, this is to large extent a subjective matter. Based on our previous experience we *define* as a measure of this uncertainty the difference between the results obtained (for the same $\Lambda_{\overline{\text{MS}}}$) in the three principal methods set out in Section 3: PMS, ECH and $\overline{\text{MS}}$. This choice is to large extent arbitrary, but as the $\overline{\text{MS}}$ RS is used in most phenomenological analyses, we adopt it for the lack of anything better. The formulae quoted below are taken from Ref. [21].

The basic quantity of interest, R_Z , defined in (1), has a nontrivial structure which mixes the effects of electroweak interactions with those of pure QCD. It can be written in the following decoupled form (i.e., for five massless flavours and the explicit m_t dependence of the expansion coefficients) as the sum of three terms with different electroweak factors [34] and separated further into four possible combinations of vector, axial vector and singlet, nonsinglet contributions:

$$\begin{aligned}
R_Z &= (R^{V,NS} + R^{A,NS}) + R^{V,S} + R^{A,S} \\
&= \sum_{i=1}^5 (g_{V,i}^2 + g_{A,i}^2) [1 + a^{(5)} + (a^{(5)})^2 r_1 + (a^{(5)})^3 r_2] \\
&\quad + \left(\sum_{i=1}^5 g_{V,i} \right)^2 [(a^{(5)})^3 s_3 + (a^{(5)})^3 s_3^{top}] \\
&\quad + \left(\frac{1}{4} \right) [(a^{(5)})^2 t_2 + (a^{(5)})^3 t_3], \tag{54}
\end{aligned}$$

where $g_{V,i} = t_{3,i} - 2Q_i \sin^2 \theta_W$, $g_{A,i} = t_{3,i}$, t_3 is the third component of the weak isospin and the sums over the electroweak coupling constants equal

$$\Gamma_1 \equiv \sum_{i=1}^5 (g_{V,i}^2 + g_{A,i}^2) = \frac{5}{2} + \frac{44}{9} \sin^4 \theta_W - \frac{14}{3} \sin^2 \theta_W = 1.6807 \pm 0.0012 \tag{55}$$

$$\Gamma_2 \equiv \left(\sum_{i=1}^5 g_{V,i} \right)^2 = \left(\frac{1}{2} + \frac{2}{3} \sin^2 \theta_W \right)^2 = 0.42850 \pm 0.00028. \tag{56}$$

The last equalities in the above relations correspond to the world average $\sin^2 \theta_W = 0.2329 \pm 0.0005$. Note that (55) implies

$$\frac{\Delta\Gamma_2}{\Gamma_2} \doteq 6.5 \cdot 10^{-4} < \frac{\Delta\Gamma_1}{\Gamma_1} \doteq 7.1 \cdot 10^{-4} \ll \frac{\Delta\Gamma_h}{\Gamma_h}, \quad (57)$$

which, combined with (5), means that the theoretical uncertainties of QCD predictions – in the square brackets in (54) – should be compared to the error of R_Z itself.

The expansion coefficients entering the above formula can be expressed as functions of the ratio $x \equiv M_z/m_t(M_Z)$, where $m_t(M_Z)$ is the renormalized, ‘running’ mass of the top quark, taken at the scale M_Z . For $n_f = 5$ and in small x expansions we have [21]:

$$\begin{aligned} r_1 &= 1.409 \\ &+ [0.065185 - 0.014815 \ln x]x \\ &+ [-0.0012311 + 0.00039683 \ln x]x^2 \\ &+ [0.000061327 - 0.000023516 \ln x]x^3 + \mathcal{O}(x^4) \end{aligned} \quad (58)$$

$$\begin{aligned} r_2 &= -12.767 \\ &+ [-0.17374 + 0.21242 \ln x - 0.037243 \ln^2 x]x \\ &+ [-0.0075218 - 0.00058859 \ln x + 0.00038305 \ln^2 x]x^2 \\ &+ [0.00050411 - 0.00012099 \ln x + 0.000031419 \ln^2 x]x^3 + \mathcal{O}(x^4) \end{aligned} \quad (59)$$

$$\begin{aligned} s_3 &= -0.41318 \\ s_3^{top} &= 0.027033x + 0.036355x^2 + 0.00058874x^3 + \mathcal{O}(x^4) \end{aligned} \quad (60)$$

$$t_2 = -3.0833 + \ln x + 0.086420x + 0.0058333x^2 + 0.00062887x^3 + \mathcal{O}(x^4) \quad (61)$$

$$\begin{aligned} t_3 &= 18.654 + 1.7222 \ln x + 1.9167 \ln^2 x \\ &+ [-0.12585 + 0.28646 \ln x - 0.011111 \ln^2 x]x \\ &+ [-0.0031322 + 0.012117 \ln x - 0.0011905 \ln^2 x]x^2 \\ &+ [-0.00088827 + 0.00047262 \ln x - 0.00017637 \ln^2 x]x^3 + \mathcal{O}(x^4). \end{aligned} \quad (62)$$

Because of different electroweak factors in front of them, each of the expressions in the square brackets of (54) is separately from the point of view of QCD RS invariant. As the optimization according to either the PMS or ECH methods does not commute with the operation of addition, the first question we have to answer is the order of these operations. In the absence of uncertainties in the values of the electroweak factors, the proper way would be first to sum all three terms in (54) and then to fix the RS. In reality, however, the errors of electroweak factors induce uncertainties in values of the coefficients multiplying powers of the QCD couplant. To optimize, in one way or another, the resulting QCD perturbative expansion (54) in such circumstances is not a well-defined exercise and we therefore have chosen to follow the opposite route. We believe that to get an estimate of the RS dependence of QCD calculations this second route is adequate. In this section we shall discuss the numerical importance of the first two terms in (54) for $m_t = 0$. The effects of non-zero m_t , as well as the third term in (54), the existence of which is also closely related to non-zero m_t , are dealt with in the next section. The second term of (54), multiplied by (56), is given at the LO only and no optimization is possible. Fortunately it contributes, in $\overline{\text{MS}}$ RS, a mere 10^{-5} to R_Z and is thus clearly negligible.

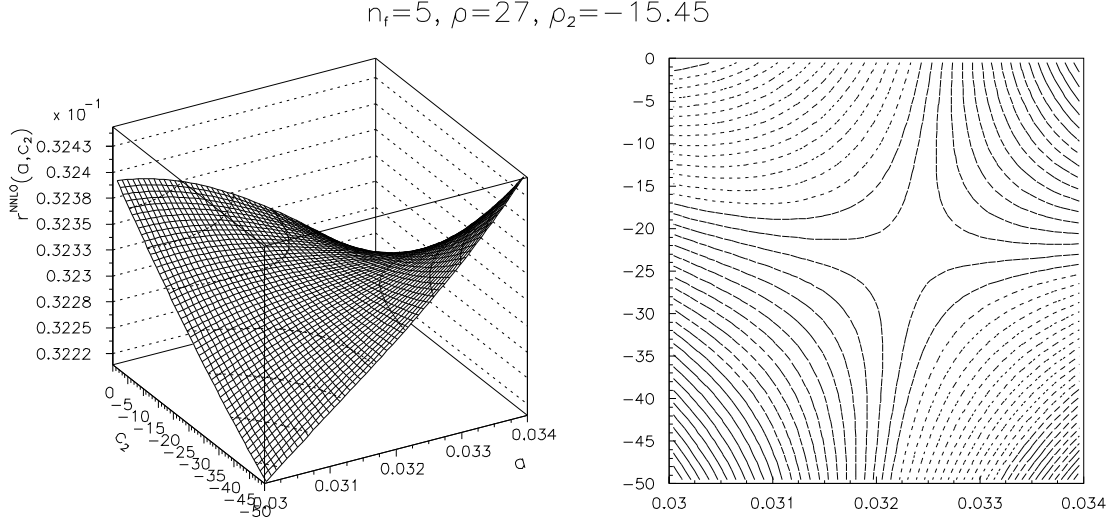


Figure 2: The NNLO approximant $r^{(3)}(a, c_2)$ in the vicinity of the saddle point for $\rho = 23$.

The dominant contribution to R_Z comes from the first term in (54). The term in the square brackets can be written as $1 + r(M_Z)$, where $r(Q)$ has exactly the form of (7) and, moreover, for massless quarks coincides with the above expression for (36) [19]. For $n_f = 5$ the crucial RG invariant $\rho_2 = -15.45$, which implies (for detailed discussion see Ref. [4]) that the saddle point of the NNLO approximant $r^{(3)}(\rho)$ will occur at the point $(a_{\text{PMS}}, c_2^{\text{PMS}})$, where $c_2^{\text{PMS}}(\rho) \rightarrow 1.5\rho_2 \doteq -23.2$. In Fig. 2 $r^{(3)}(\rho = 27)$ is plotted as a function of a, c_2 near this saddle point, together with the contours of the constant $r^{(3)}$. We have calculated the NLO as well as the NNLO approximants of the quantity in the first square bracket of (54), with the unity subtracted, in the three chosen RSs and in the interval $\rho \in (18, 28)$, which corresponds to the measured value of $M_Z \doteq 91.4$ GeV and $\Lambda_{\overline{\text{MS}}}^{(5)}$ in the interval $\Lambda_{\overline{\text{MS}}}^{(5)} \in (50, 500)$ MeV. As the differences are tiny we normalize all our results to the NLO result in the conventional $\overline{\text{MS}}$ RS, and plot the relative difference,

$$r_\rho \equiv \frac{r^{(i)}(\text{RS})}{r^{\text{NLO}}(\Lambda_{\overline{\text{MS}}})} - 1, \quad (63)$$

where $i = \text{NLO, NNLO}$ and $\text{RS} = \text{PMS, ECH}$ or $\overline{\text{MS}}$. We draw the following conclusion from Fig. 3:

1. The differences between PMS and ECH approaches are minuscule, about 0.1% at the NLO and totally negligible at the NNLO,
2. the difference between the PMS (or ECH) and $\overline{\text{MS}}$ approaches is
 - about 0.7% at the NLO and
 - about 0.3% at the NNLO (this comes from the ratio of the dotted and dash-dotted curves in Fig. 3). This documents the trend, observed in earlier works, that inclusion of the NNLO corrections diminishes the RS dependences and thus decreases the theoretical uncertainty.

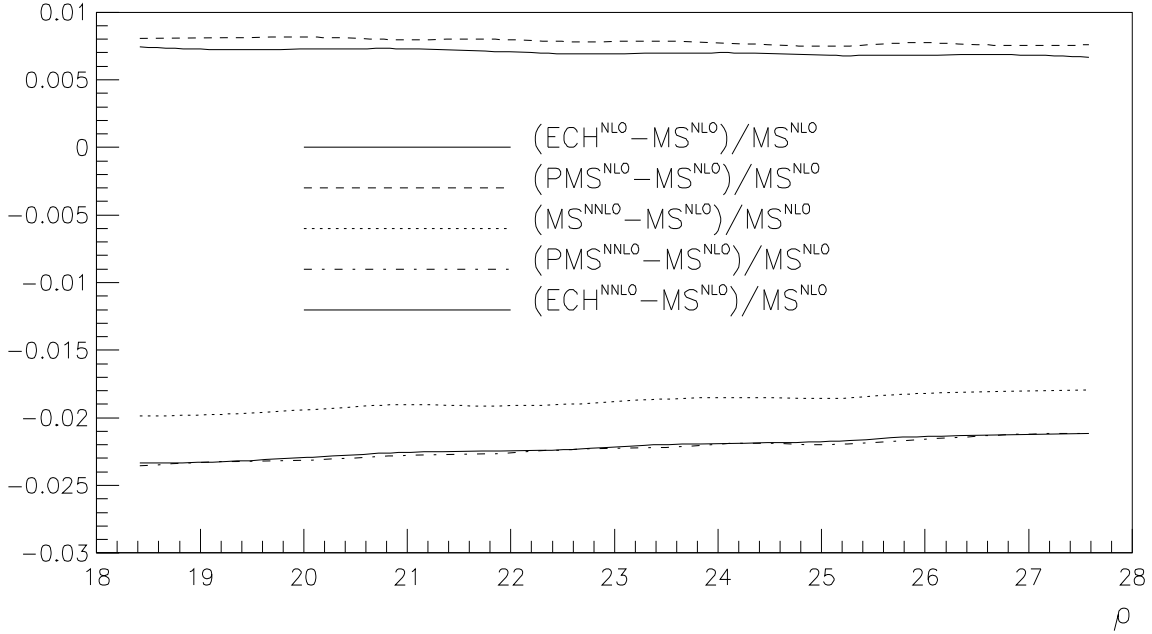


Figure 3: The ratio r_ρ , defined in the text.

3. the differences between the NLO and NNLO approximations amount to about 2% in the $\overline{\text{MS}}$ RS (as already estimated in Section 3) and to about 3% for PMS (or ECH).

Given the current precision of the data (5), which translates into 8.5% accuracy on the couplant $a(M_Z)$, this implies that none of the mentioned differences is discernible. Moreover, only the last difference, namely the effect of including the NNLO correction, has any chance of being seen in the data, but even this would require at least a factor three improvement in the precision of Γ_h .

5 The dependence of R_Z on m_b and m_t

As already pointed out, massive quarks complicate the consistency conditions, discussed in Section 2, as their renormalized masses also ‘run’ and there is so far no generalization of the relations (19) available. We therefore estimate the effects of non-zero top and bottom quark masses within the $\overline{\text{MS}}$ RS. Recall that (54) are expansions in $a^{(5)}$ corresponding to five massless quarks, and thus all effects of finite m_b and m_t are contained in the expansion coefficients.

First we deal with the effects of the finite $x = M_Z/m_t$ in the first and third term of (54). In the first case the x -dependent terms of r_1 and r_2 vanish in the limit $x \rightarrow 0$ and the leading, constant, ones correspond to $n_f = 5$ in accordance with the decoupling theorem [35]. For $x = 0.4225$, corresponding to $M_Z = 91.187$ and $m_t(M_Z) = 140$ GeV, as suggested in Ref. [21], $R^{V,NS} + R^{A,NS}$ changes by the factor $3.7 \cdot 10^{-5}$, which is an effect two orders of magnitude smaller than the experimental error of R_Z , estimated in (5), and one order of magnitude smaller than the effects discussed in the preceding section. It can therefore be safely neglected.

The contribution of the last term in (54), coming from the axial vector, flavour singlet

channel, where the familiar axial anomaly operates, is numerically nonnegligible. Despite the fact that the leading terms in t_2 and t_3 are x -independent, the nonvanishing of $R^{A,S}$ is due to non-zero m_t , or, more precisely, to the effect of the difference $m_t - m_b$ ⁹. This comes from the fact that axial couplings of quarks in weak doublets are opposite and, apart from mass effects, their contributions cancel. Consequently, for $m_t = 0$ both t_2 and t_3 , and thereby also $R^{A,S}$, must vanish. The fact that this vanishing is not obvious in the small x expansions of (54) is not surprising, as $m_t \rightarrow 0$ corresponds on the contrary to $x \rightarrow \infty$. Note that the presence of powers of $\ln x$ in the coefficients t_2 and t_3 implies that a resummation of these logarithms is necessary [32] even in the limit $x \rightarrow 0$. As the contribution $R^{A,S}$ can be interpreted as the top quark mass effect, we again determine its contribution in the $\overline{\text{MS}}$ RS only. For $m_t(M_Z) = 140$ GeV, $R^{A,S} = -0.00160$.

The effects of finite value of m_b/M_Z have been studied in detail in [33]. Here we merely recall the form and numerical values of the leading contributions in the vector and axial vector, nonsinglet $b\bar{b}$ channels resulting from these effects:

$$R_b^{V,NS} \equiv g_{V,b}^2 \left(1 + \left[1 + 12 \frac{m_b^2(M_Z)}{M_Z^2} \right] a^{(5)}(M_Z) + \mathcal{O}([a^{(5)}]^2) \right), \quad (64)$$

$$R_b^{A,NS} \equiv g_{A,b}^2 \left(1 - 6 \frac{m_b^2(M_Z)}{M_Z^2} + \mathcal{O}(a^{(5)}) \right). \quad (65)$$

For $m_b(M_Z) = 4.8$ [33] and $a^{(5)}(M_Z) = 0.037$ the leading m_b/M_Z contribution to R_Z coming from the axial channel thus amounts to $4.2 \cdot 10^{-3}$, whereas in the vector channel we get a mere $1.5 \cdot 10^{-4}$.

6 The estimate of the still higher order terms

As we saw in the preceding two sections, the NNLO corrections to Γ_h are, compared to experimental accuracy of its measurement, tiny effects, and so it seems reasonably safe to stop at this order. On the other hand it is generally accepted that perturbative series in QCD do not converge, but represent merely asymptotic expansions to the full result. In such situation it is certainly useful to have at least some estimate of the magnitude of the so far uncalculated (and in the near future uncalculable) higher orders.

An attempt in this direction has recently been made in [37], using the so-called ‘improvement formula’ of Ref. [2], which represents an approximation of the PMS optimization discussed in subsection 2.3. Its essence is to reexpand the PMS result optimized to the Nth order in powers of the couplant in any fixed RS¹⁰ and take the coefficient of this expansion at the (N+1)th order as an estimate of its true value. Instead of the PMS approach the ECH one of subsection 2.4 can be equally well used for this purpose. The resulting estimates are only slightly different.

Here we outline the main steps of this method for the quantity (36), closely related to Γ_h . Consider first the Nth order partial sum of the perturbative expansion for a physical

⁹An alternative interpretation of this effect is discussed in Ref. [36].

¹⁰The optimized result is, of course, independent of the choice of this RS and is constructed from quantities up to the Nth order only.

quantity D^{11} :

$$D_N = \sum_{i=0}^{N-1} d_i a^{i+1}. \quad (66)$$

Carrying out the optimization of (66) according to either the PMS or ECH approaches leads to the optimized result, denoted below as $D_N^{\text{opt}}(a_{\text{opt}})$. If we now reexpand $D_N^{\text{opt}}(a_{\text{opt}})$ in terms of the couplant $a(\text{RS})$ in a chosen RS ¹² we find

$$D_N^{\text{opt}}(a_{\text{opt}}) = D_N(a) + \delta D_N^{\text{opt}} a^{N+1}, \quad (67)$$

where

$$\delta D_N^{\text{opt}} = \Omega_N(d_i, c_i) - \Omega_N(d_i^{\text{opt}}, c_i^{\text{opt}}) \quad (68)$$

give, according to ref. [37], the estimate of the coefficient d_N in the chosen RS. For the three lowest orders the functions $\Omega_N(d_i, c_i)$ are given as [37]:

$$\begin{aligned} \Omega_2 &= d_0 d_1 (c_1 + d_1) \\ \Omega_3 &= d_0 d_1 (c_2 - \frac{1}{2} c_1 d_1 - 2d_1^2 + 3d_2) \\ \Omega_4 &= \frac{d_0}{3} (3c_3 d_1 + c_2 d_2 - 4c_2 d_1^2 + 2c_1 d_1 d_2 - c_1 d_3 \\ &\quad + 14d_1^4 - 28d_1^2 d_2 + 5d_2^2 + 12d_1 d_3). \end{aligned} \quad (69)$$

These formulae can be derived from the following exact equations relating Ω_j to the coefficients d_j, c_j and the RG invariants ρ_j :

$$d_j = \frac{\rho_j}{j-1} - \frac{c_j}{j-1} + \frac{\Omega_j}{d_0}. \quad (70)$$

Note that in order to evaluate Ω_j only d_i, c_i at lower orders $i \leq j-1$ are actually needed!

If the ECH approach is used for the optimization, the formulae (68) is particularly simple as $d_i^{\text{opt}} = 0$ by definition and thus

$$\begin{aligned} \delta D_2^{\text{ECH}} &= \Omega_2(d_1, c_1) \\ \delta D_3^{\text{ECH}} &= \Omega_3(d_1, d_2, c_1, c_2) \\ \delta D_4^{\text{ECH}} &= \Omega_4(d_1, d_2, d_3, c_1, c_2, c_3). \end{aligned} \quad (71)$$

The estimate (71) is thus equivalent to the assumption that d_N is dominated by the last term in (70). Extensive discussion of this assumption and its consequences is given in Ref. [37] and is also related to Ref. [38].

Using the PMS approach the resulting estimate of d_N differs from (71) by the presence of the second term in (68), which does not vanish as in the ECH approach. However, it was shown in ref. [37] that $\Omega_2(d_i^{\text{PMS}}, c_i^{\text{PMS}})$ and $\Omega_4(d_i^{\text{PMS}}, c_i^{\text{PMS}})$ are small and $\Omega_3(d_i^{\text{PMS}}, c_i^{\text{PMS}}) = 0$. In the following numerical estimates only the ECH-based results are therefore presented.

¹¹In this section we drop the specification of the number of quark flavours in the couplant a .

¹²The magnitude and therefore also the estimate of higher order coefficients depends on the choice of RS. We drop the argument ‘RS’ of $a(\text{RS})$ here.

n_f	r_2^{exact}	$r_2^{estimate}$	r_3^{est}	$r_4^{estimate} - c_3 r_1$
1	-7.84	-14.41	-166	-1750
2	-9.04	-12.65	-147	-1161
3	-10.27	-11.04	-128	-668
4	-11.52	-9.59	-112	-263
5	-12.76	-8.32	-97	67
6	-14.01	-7.19	-83	330

Table 1: The estimate of the so far uncalculated higher order coefficients for the quantity $R(s)$ in the $\overline{\text{MS}}$ RS and using the ECH optimization procedure.

There is one subtle point in the derivation of estimates for higher order coefficients r_k of time-like quantities like (1) or (36). For instance, $R(s)$ of (36) is related to the so-called D -function $D(Q^2)$, defined primarily in the Euclidean region, via the dispersion relation

$$D(Q^2) = Q^2 \int_0^\infty \frac{R(s)}{(s + Q^2)^2} ds. \quad (72)$$

The knowledge of $R(s)$ is in principle equivalent to that of $D(Q^2)$, but as most of the optimization procedures or methods of higher order estimates do not commute with the functional on the r.h.s. of (72), we face the question as to which quantity to apply Eq.(71). This nontrivial problem is discussed in Ref. [37], the conclusion being that they should be applied to the quantities in the Euclidean region –, for instance, $D(Q^2)$. Having obtained the estimates for higher order coefficients d_j , the corresponding estimates for the coefficients r_j of $R(s)$ follow from the relations

$$\begin{aligned} r_1 &= d_1 \\ r_2 &= d_2 - \frac{\pi^2 b^2}{12}, \\ r_3 &= d_3 - \frac{\pi^2 b^2}{4} \\ r_4 &= d_4 - \frac{\pi^2 b^2}{4} (2d_2 + \frac{7}{3}c_1 d_1 + \frac{1}{2}c_1^2 + c_2) + \frac{\pi^4 b^4}{80}. \end{aligned} \quad (73)$$

The terms, proportional to powers of π^2 , come from the analytical continuation of the couplant $a(\mu)$ from the Euclidean region, where $\mu^2 < 0$ to the Minkowskean one, where $\mu^2 > 0$. Taking into account the fact that in the $\overline{\text{MS}}$ RS we have [39]:

$$\begin{aligned} d_1(\overline{\text{MS}}) &\approx 1.986 - 0.115n_f \\ d_2(\overline{\text{MS}}) &\approx 18.244 - 4.216n_f + 0.086n_f^2 \end{aligned} \quad (74)$$

$$c_2(\overline{\text{MS}}) = \frac{77139 - 15099n_f + 325n_f^2}{9504 - 576n_f}, \quad (75)$$

and using (71) we get the estimates, obtained originally in Ref. [37], summarized in Table 2 and valid for the $\overline{\text{MS}}$ RS.¹³ In order to get some feeling of the possible accuracy of these

¹³Neglecting the terms of the light-by-light type, which violate the structure of (36).

estimates the above table also includes the results for the NNLO coefficient r_2 , for which the exact calculations are available. In the case of the coefficient r_4 , only the estimate for the combination $r_4 - r_1 c_3$ is presented, as the four loop β -function coefficient $c_3(\overline{\text{MS}})$ is so far unknown.

As the dominant contribution to (1) comes from the nonsinglet channel – first term of (54) –, the above estimates are relevant for this quantity as well. For $a(\overline{\text{MS}}, M_Z) = 0.037$, $n_f = 5$ and using the estimates of Table 1, we find that the terms $r_3 a^4$ and $r_4 a^5$ contribute approximately $-3 \cdot 10^{-4}$ and $8 \cdot 10^{-6}$ respectively¹⁴. Note that while the latter contribution is entirely negligible, the former is of the same order as the RS uncertainty of the NNLO contribution.

7 Summary and conclusions

In the preceding sections we have analyzed various contributions to, and theoretical uncertainties of, the quantity (1). The results of these analyses are summarized in Table 2. All these numbers should be contrasted with the current experimental error of R_Z , which is $5.9 \cdot 10^{-3}$. We see that there is a number of affects that are comparable to the current experimental accuracy of R_Z , the most important of them being the NLO perturbative correction and, interestingly, the effects of finite b quark mass correction to the Born term in the axial channel. This, however, has nothing to do with QCD. On the other the hand, the data are not yet sufficiently precise to be sensitive to, for instance, the NNLO perturbative correction. Further improvement in the measurement of Γ_h is clearly very desirable.

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¹⁴For the latter contribution the additional assumption, concerning $c_3(\overline{\text{MS}})$, had been made: $c_3 = c_2^2/c$.

	type of contribution	contributes to R_Z
1	LO nonsinglet channel	$+62.2 \cdot 10^{-3}$
2	NLO nonsinglet channel	$+3.24 \cdot 10^{-3}$
3	NNLO nonsinglet channel	$-1.08 \cdot 10^{-3}$
4	N ³ LO nonsinglet channel	$-5.1 \cdot 10^{-4}$
5	N ⁴ LO nonsinglet channel	$+1.3 \cdot 10^{-5}$
6	m_t in nonsinglet channel	$+3.7 \cdot 10^{-5}$
7	m_t in singlet channel	$-1.6 \cdot 10^{-3}$
8	smooth thresholds in α_s	$+1.3 \cdot 10^{-3}$
9	m_b effects in Born term, axial channel	$-4.2 \cdot 10^{-3}$
10	m_b effects in LO term, vector channel	$+1.5 \cdot 10^{-4}$
11	RS uncertainty at NLO	$-4.7 \cdot 10^{-4}$
12	RS uncertainty at NNLO	$-2.1 \cdot 10^{-4}$
13	experimental error	$\pm 5.9 \cdot 10^{-3}$

Table 2: Summary of various contributions to, and uncertainties of, R_Z . All numbers, except items 8,11,12 are correspond to $\overline{\text{MS}}$ RS.

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